Full wwPDB X-ray Structure Validation Report (i)

Aug 22, 2026 – 03:19 am BST

PDB ID	:	2C3P / pdb_00002c3p
Title	:	CRYSTAL STRUCTURE OF THE FREE RADICAL INTERMEDIATE OF PYRUVATE:FERREDOXIN OXIDOREDUCTASE FROM Desulfovibrio africanus
Authors	:	Cavazza, C.; Contreras-Martel, C.; Pieulle, L.; Chabriere, E.; Hatchikian, E.C.; Fontecilla-Camps, J.C.
Deposited on	:	2005-10-11
Resolution	:	2.33 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) were used in the production of this report:

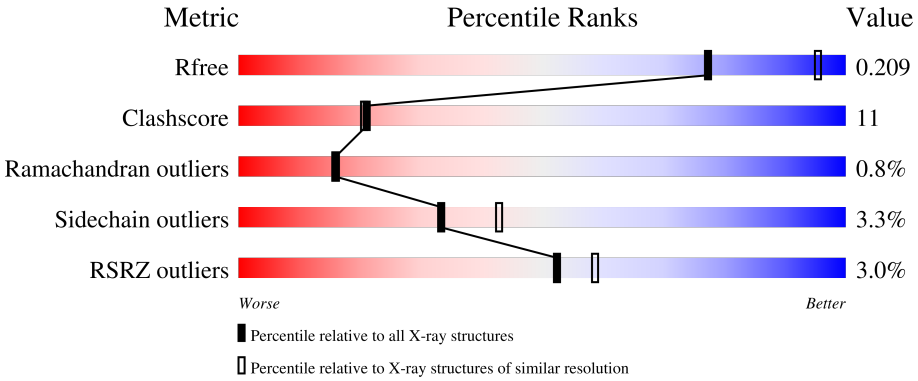
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.33 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	3031 (2.36-2.32)
Clashscore	190562	3127 (2.36-2.32)
Ramachandran outliers	187476	3095 (2.36-2.32)
Sidechain outliers	187428	3095 (2.36-2.32)
RSRZ outliers	180081	3033 (2.36-2.32)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1231	3% 71% 25%
1	B	1231	2% 80% 18%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	1TP	A	2236	X	-	-	-
3	1TP	B	2236	X	-	-	-

2 Entry composition

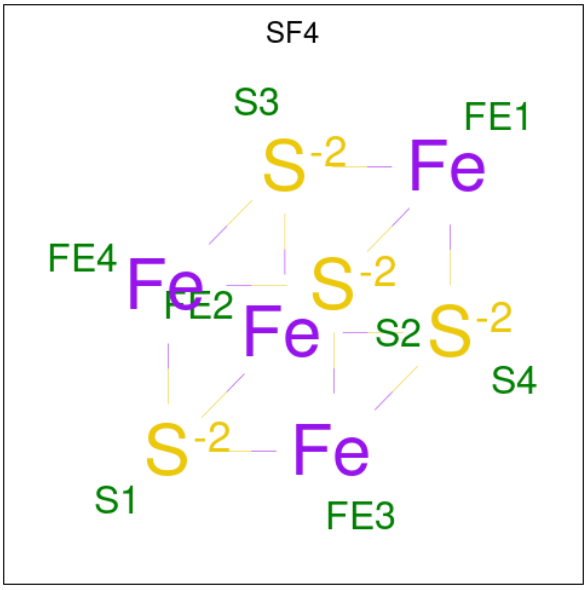
There are 6 unique types of molecules in this entry. The entry contains 19733 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called PYRUVATE-FERREDOXIN OXIDOREDUCTASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1231	Total	C	N	O	S	0	0	0
			9383	5941	1599	1784	59			
1	B	1231	Total	C	N	O	S	0	0	0
			9383	5941	1599	1784	59			

- Molecule 2 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



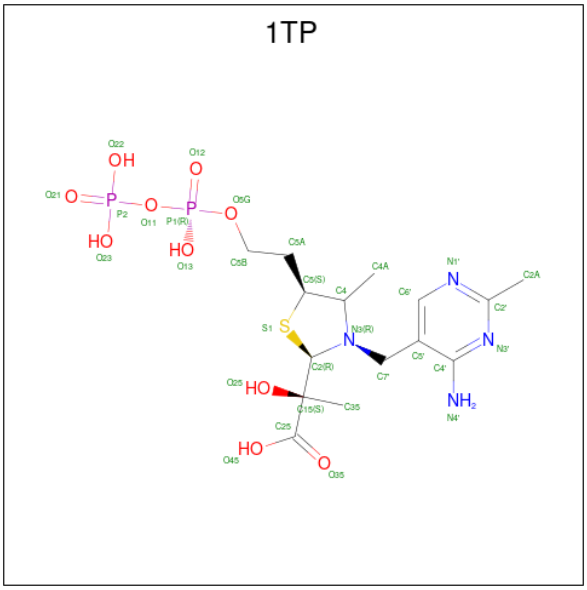
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	Fe	S		0	0
			8	4	4			
2	A	1	Total	Fe	S		0	0
			8	4	4			
2	A	1	Total	Fe	S		0	0
			8	4	4			
2	B	1	Total	Fe	S		0	0
			8	4	4			

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	1	Total Fe S 8 4 4	0	0
2	B	1	Total Fe S 8 4 4	0	0

- Molecule 3 is 1-(2-{(2S,4R,5R)-3-[(4-AMINO-2-METHYLPYRIMIDIN-5-YL)METHYL]-2-[(1S)-1-CARBOXY-1-HYDROXYETHYL]-4-METHYL-1,3-THIAZOLIDIN-5-YL}ETHOXY)-1,1,3,3-TETRAHYDROXY-1LAMBDA 5 -DIPHOSPHOX-1-EN-2-IUM 3-OXIDE (CCD ID: 1TP) (formula: $C_{15}H_{26}N_4O_{10}P_2S$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C N O P S 32 15 4 10 2 1	0	0
3	B	1	Total C N O P S 32 15 4 10 2 1	0	0

- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total Mg 1 1	0	0
4	B	1	Total Mg 1 1	0	0

- Molecule 5 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total Ca 1 1	0	0
5	B	1	Total Ca 1 1	0	0

- Molecule 6 is water.

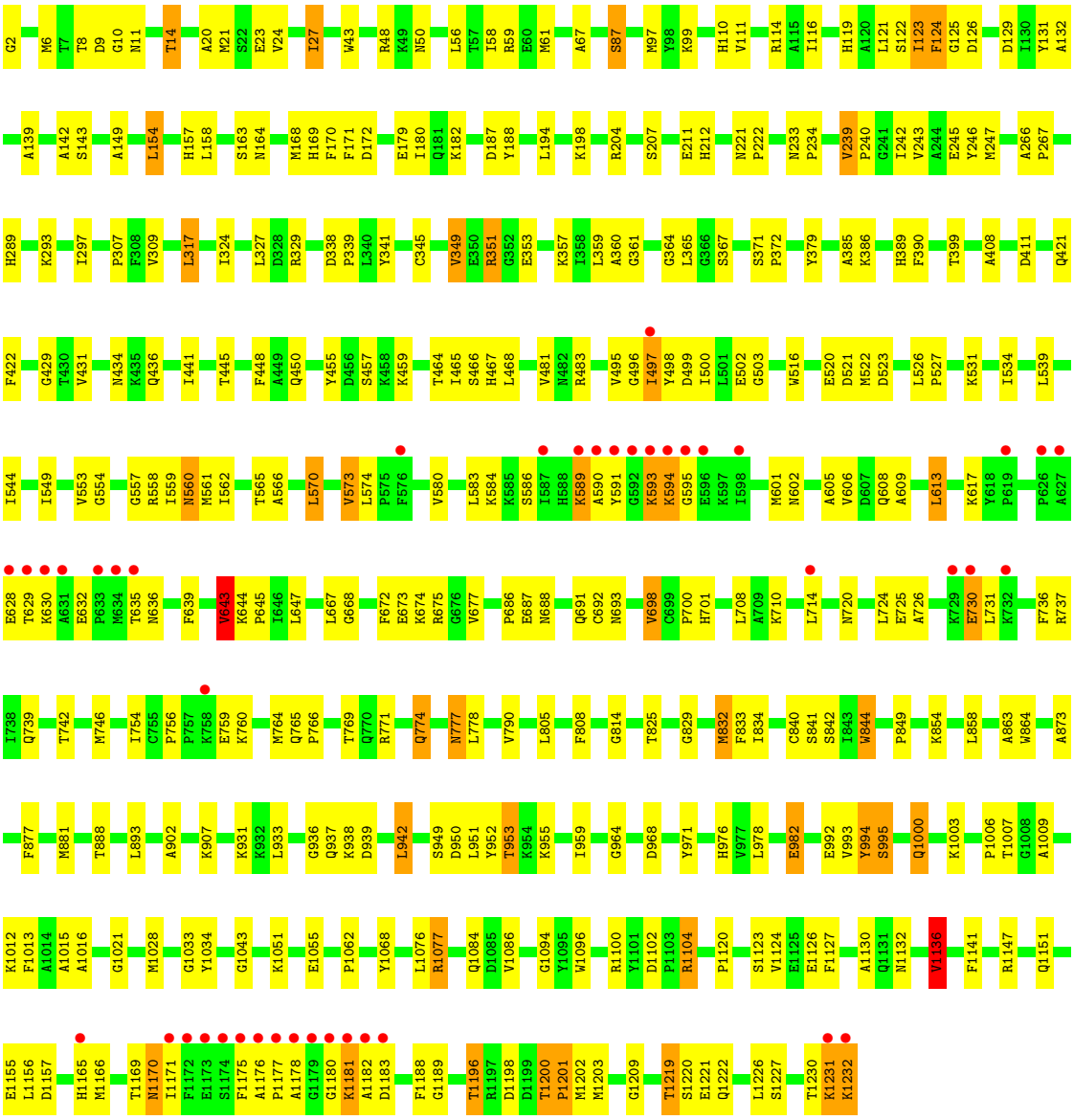
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	379	Total O 379 379	0	0
6	B	472	Total O 472 472	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

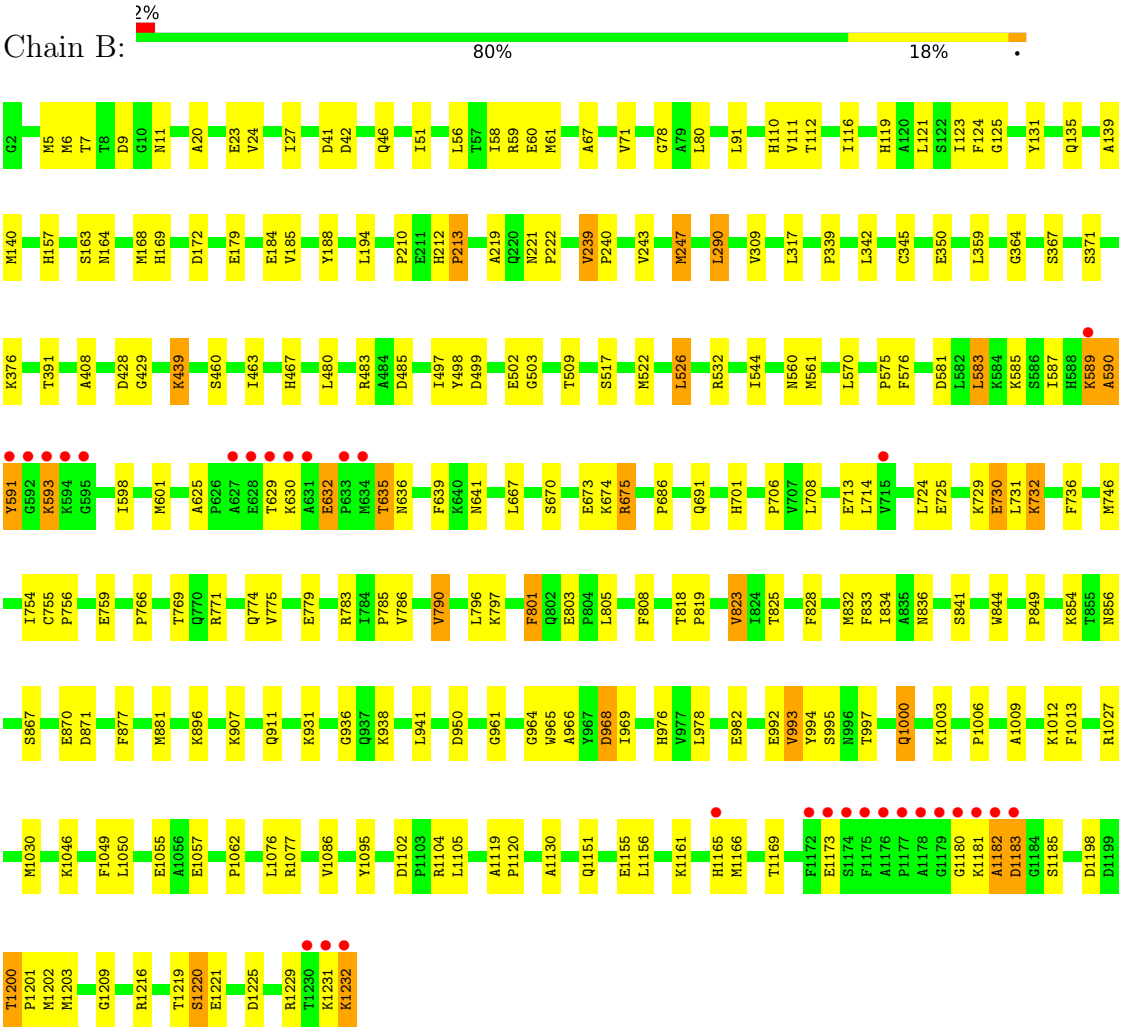
• Molecule 1: PYRUVATE-FERREDOXIN OXIDOREDUCTASE

Chain A: 



• Molecule 1: PYRUVATE-FERREDOXIN OXIDOREDUCTASE

Chain B:


2%
80%
18%
G2 M5 M6 T7 T8 D9 G10 N11 A20 E23 V24 I27 D41 D42 Q46 I51 L56 T57 I58 R59 E60 M61 A67 V71 G78 A79 L80 L91 H110 V111 T112 I116 H119 A120 L121 S122 I123 F124 G125 Y131 Q135 A139
M140 H157 S163 N164 M168 H169 D172 E179 E184 V185 Y188 L194 P210 E211 H212 P213 A219 Q220 N221 P222 V239 P240 V243 M247 L290 V309 L317 P339 L342 C345 E350 L359 G364 S367 S371
K376 T391 A408 D428 G429 K439 S460 I463 H467 L480 R483 A484 D485 I497 Y498 D499 E502 G503 T509 S517 M522 L526 R532 I544 N560 M561 L570 P575 F576 D581 L582 L583 K584 K585 S586 I587 H588 K589 A590
Y591 G592 K593 K594 G595 I598 M601 A625 P626 A627 E628 T629 K630 A631 E632 P633 M634 T635 N636 F639 K640 N641 L667 S670 E673 K674 R675 P686 Q691 H701 P706 V707 L708 E713 L714 V715 L724 E725 K729 E730 L731 K732 F736 M746
I754 C755 P756 E759 P766 T769 Q770 R771 Q774 V775 E779 R783 I784 P785 V786 V790 L796 K797 F801 Q802 E803 P804 L805 F808 T818 P819 V823 I824 T825 F828 M832 F833 I834 A835 N836 S841 W844 P849 K854 T855 N856
S867 E870 D871 F877 M881 K896 K907 Q911 K931 G936 Q937 K938 L941 D950 G961 G964 W965 A966 Y967 D968 I969 H976 V977 L978 E982 E992 V993 Y994 S995 N996 T997 Q1000 K1003 P1006 A1009 K1012 F1013 R1027
M1030 K1046 F1049 L1050 E1055 A1056 E1057 P1062 L1076 R1077 V1086 Y1095 D1102 P1103 R1104 L1105 A1119 P1120 A1130 Q1151 E1155 L1156 K1161 H1165 M1166 T1169 F1172 E1173 S1174 F1175 A1176 P1177 A1178 G1179 G1180 K1181 A1182 D1183 G1184 S1185 D1198 D1199
T1200 P1201 M1202 M1203 G1209 R1216 T1219 S1220 E1221 D1225 R1229 T1230 K1231 K1232

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	85.97Å 145.84Å 210.82Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.37 – 2.33 47.37 – 2.33	Depositor EDS
% Data completeness (in resolution range)	98.3 (47.37-2.33) 98.4 (47.37-2.33)	Depositor EDS
R_{merge}	0.01	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.55 (at 2.34Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.171 , 0.223 0.158 , 0.209	Depositor DCC
R_{free} test set	5637 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å^2)	20.5	Xtriage
Anisotropy	0.182	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 47.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	19733	wwPDB-VP
Average B, all atoms (Å^2)	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.88% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 1TP, SF4, CA, MG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.53	1/9585 (0.0%)	1.01	55/12954 (0.4%)
1	B	0.56	0/9585	1.02	45/12954 (0.3%)
All	All	0.55	1/19170 (0.0%)	1.02	100/25908 (0.4%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	239	VAL	CA-CB	5.92	1.57	1.53

All (100) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	125	GLY	N-CA-C	10.37	129.41	111.15
1	B	125	GLY	N-CA-C	9.42	127.73	111.15
1	A	756	PRO	N-CA-C	8.63	121.23	110.70
1	B	993	VAL	CB-CA-C	-8.43	103.82	111.74
1	B	771	ARG	N-CA-C	8.35	120.01	111.07
1	B	790	VAL	N-CA-C	8.19	118.23	110.53
1	B	756	PRO	N-CA-C	8.09	120.57	110.70
1	B	590	ALA	N-CA-C	-8.01	100.56	110.41
1	A	497	ILE	N-CA-C	7.95	120.00	111.58
1	A	27	ILE	N-CA-C	7.91	120.34	108.80
1	B	364	GLY	N-CA-C	7.63	125.97	114.61
1	A	124	PHE	N-CA-C	7.48	120.18	110.53
1	B	593	LYS	N-CA-C	-6.85	104.80	113.02
1	A	771	ARG	N-CA-C	6.85	118.40	111.07
1	A	1016	ALA	N-CA-C	-6.83	103.31	112.94
1	B	994	TYR	N-CA-C	-6.77	96.58	108.23
1	B	969	ILE	N-CA-C	6.67	116.82	110.42
1	B	408	ALA	N-CA-C	-6.63	105.19	113.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	774	GLN	N-CA-C	6.62	120.61	112.54
1	A	863	ALA	N-CA-C	-6.58	97.81	108.41
1	A	500	ILE	N-CA-C	6.55	119.28	111.09
1	B	139	ALA	N-CA-C	-6.55	100.79	110.48
1	A	774	GLN	N-CA-C	6.50	120.42	112.23
1	A	668	GLY	N-CA-C	6.45	124.84	114.90
1	B	517	SER	N-CA-C	6.36	118.29	111.36
1	A	833	PHE	N-CA-C	-6.35	99.37	109.59
1	B	213	PRO	N-CA-C	6.35	120.93	111.41
1	B	570	LEU	N-CA-C	6.35	121.97	113.72
1	A	559	ILE	N-CA-C	6.32	121.73	113.07
1	B	755	CYS	CA-C-N	6.28	126.84	120.38
1	B	755	CYS	C-N-CA	6.28	126.84	120.38
1	B	966	ALA	N-CA-C	6.27	118.11	111.28
1	A	1136	VAL	CB-CA-C	-6.17	103.80	112.14
1	A	1077	ARG	N-CA-C	6.08	118.68	111.33
1	A	643	VAL	N-CA-C	6.06	116.84	110.72
1	B	1220	SER	N-CA-C	-6.04	104.60	111.07
1	A	338	ASP	CA-C-N	5.97	127.30	119.84
1	A	338	ASP	C-N-CA	5.97	127.30	119.84
1	B	576	PHE	N-CA-C	5.96	121.14	111.37
1	A	710	LYS	N-CA-C	-5.96	101.19	110.42
1	A	23	GLU	N-CA-C	-5.84	106.69	113.88
1	B	78	GLY	N-CA-C	5.84	124.07	115.08
1	B	239	VAL	CB-CA-C	-5.83	108.17	113.70
1	A	123	ILE	N-CA-C	-5.79	106.14	112.80
1	A	139	ALA	N-CA-C	-5.79	101.92	110.48
1	A	111	VAL	N-CA-C	5.70	116.09	108.11
1	A	844	TRP	N-CA-C	-5.70	105.83	112.89
1	A	1201	PRO	N-CA-C	-5.68	106.76	113.86
1	A	742	THR	N-CA-C	5.67	118.23	111.71
1	B	219	ALA	N-CA-C	-5.65	99.98	109.07
1	B	870	GLU	N-CA-C	5.62	119.99	113.18
1	A	832	MET	N-CA-C	5.61	118.87	109.95
1	A	570	LEU	N-CA-C	5.59	120.38	113.50
1	B	485	ASP	N-CA-C	-5.57	106.32	113.23
1	A	888	THR	N-CA-C	-5.56	105.37	111.82
1	A	457	SER	N-CA-C	-5.56	105.76	112.54
1	B	575	PRO	N-CA-C	-5.56	102.40	111.68
1	A	675	ARG	N-CA-C	5.55	117.33	111.28
1	A	21	MET	N-CA-C	5.54	120.03	113.16
1	B	119	HIS	N-CA-C	-5.50	105.83	112.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	172	ASP	N-CA-C	5.49	118.15	109.96
1	B	801	PHE	N-CA-C	-5.49	106.16	112.92
1	B	968	ASP	N-CA-C	5.48	116.84	108.30
1	B	23	GLU	N-CA-C	-5.47	107.15	113.88
1	B	818	THR	N-CA-C	5.45	121.09	113.57
1	A	1141	PHE	CA-C-N	5.44	125.52	119.32
1	A	1141	PHE	C-N-CA	5.44	125.52	119.32
1	B	759	GLU	N-CA-C	-5.42	98.92	108.23
1	B	833	PHE	N-CA-C	-5.41	101.34	109.95
1	B	589	LYS	N-CA-C	-5.41	105.02	111.03
1	B	111	VAL	N-CA-C	5.40	115.67	108.11
1	A	119	HIS	N-CA-C	-5.35	106.02	112.54
1	A	726	ALA	N-CA-C	5.35	118.10	110.24
1	B	641	ASN	N-CA-C	5.35	119.86	113.23
1	A	143	SER	N-CA-C	-5.28	100.80	109.40
1	A	995	SER	N-CA-C	5.26	116.87	111.03
1	A	172	ASP	N-CA-C	5.25	117.84	109.96
1	A	1170	ASN	N-CA-C	-5.25	106.82	114.12
1	B	247	MET	N-CA-C	-5.24	105.57	111.28
1	A	408	ALA	N-CA-C	-5.15	106.77	113.16
1	A	364	GLY	N-CA-C	5.14	125.36	113.18
1	A	778	LEU	N-CA-C	-5.14	105.75	111.36
1	A	182	LYS	N-CA-C	-5.14	101.38	109.25
1	B	391	THR	N-CA-C	-5.14	101.49	109.72
1	B	675	ARG	N-CA-C	5.11	117.59	111.71
1	A	725	GLU	N-CA-C	-5.10	101.64	109.76
1	A	448	PHE	N-CA-C	-5.10	101.39	109.96
1	A	760	LYS	N-CA-C	5.10	117.49	110.35
1	A	560	ASN	N-CA-C	5.09	117.22	111.11
1	B	1200	THR	N-CA-C	5.08	117.09	110.08
1	A	994	TYR	N-CA-C	-5.06	99.08	107.99
1	A	864	TRP	N-CA-C	5.06	117.22	109.07
1	B	371	SER	N-CA-C	5.06	116.38	110.31
1	A	698	VAL	N-CA-C	5.05	119.52	112.50
1	A	1200	THR	N-CA-C	5.04	117.96	110.39
1	A	933	LEU	N-CA-C	5.04	117.51	111.71
1	B	706	PRO	N-CA-C	-5.04	103.27	111.19
1	A	207	SER	N-CA-C	5.04	116.61	110.41
1	A	842	SER	N-CA-C	-5.02	106.32	112.90
1	B	560	ASN	N-CA-C	5.00	117.11	111.11

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	9383	0	9262	257	0
1	B	9383	0	9262	178	0
2	A	24	0	0	0	0
2	B	24	0	0	0	0
3	A	32	0	21	7	0
3	B	32	0	21	8	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
6	A	379	0	0	3	0
6	B	472	0	0	7	0
All	All	19733	0	18566	413	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 11.

All (413) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:2236:1TP:C25	3:A:2236:1TP:C15	1.79	1.59
3:B:2236:1TP:C25	3:B:2236:1TP:C15	1.82	1.56
3:B:2236:1TP:C2	3:B:2236:1TP:N3	1.67	1.48
3:B:2236:1TP:C15	3:B:2236:1TP:C2	1.93	1.44
3:A:2236:1TP:C15	3:A:2236:1TP:C2	2.09	1.29
1:B:1200:THR:HG22	1:B:1202:MET:H	1.17	1.07
1:A:1200:THR:HG22	1:A:1202:MET:H	1.25	1.02
1:A:639:PHE:HA	1:A:643:VAL:HG13	1.41	1.00
1:A:1200:THR:HG23	1:A:1202:MET:HE3	1.48	0.95
1:A:1231:LYS:HG3	1:A:1232:LYS:H	1.33	0.93
1:A:635:THR:HG22	1:A:636:ASN:H	1.35	0.90
1:A:877:PHE:HE1	1:A:982:GLU:HG3	1.36	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:554:GLY:HA3	1:A:601:MET:HE2	1.52	0.89
1:B:110:HIS:HD2	1:B:169:HIS:CD2	1.92	0.88
1:B:1200:THR:HG23	1:B:1202:MET:HE3	1.57	0.85
1:A:1132:ASN:O	1:A:1136:VAL:HG22	1.77	0.85
3:A:2236:1TP:C15	3:A:2236:1TP:H2	2.06	0.85
1:B:1200:THR:HG22	1:B:1202:MET:N	1.91	0.85
1:B:877:PHE:HE1	1:B:982:GLU:HG3	1.39	0.84
1:B:110:HIS:HD2	1:B:169:HIS:HD2	1.20	0.84
1:A:566:ALA:HA	1:A:613:LEU:HD21	1.60	0.83
1:A:27:ILE:HD11	1:A:1013:PHE:CE2	2.15	0.82
1:A:1200:THR:HG22	1:A:1202:MET:N	1.93	0.82
1:B:110:HIS:CD2	1:B:169:HIS:HD2	1.97	0.82
1:A:110:HIS:HD2	1:A:169:HIS:HD2	1.28	0.81
1:B:877:PHE:CE1	1:B:982:GLU:HG3	2.16	0.81
1:A:1076:LEU:HD13	1:A:1086:VAL:HG21	1.63	0.81
1:B:731:LEU:CD2	1:B:790:VAL:HG11	2.11	0.80
1:B:635:THR:HG23	1:B:639:PHE:HB3	1.64	0.80
1:B:1151:GLN:O	1:B:1155:GLU:HG3	1.81	0.80
1:B:561:MET:HE1	1:B:583:LEU:HD21	1.62	0.80
1:A:1151:GLN:O	1:A:1155:GLU:HG3	1.83	0.78
1:A:1200:THR:CG2	1:A:1202:MET:HE3	2.13	0.78
1:A:544:ILE:HD12	1:A:613:LEU:HD13	1.65	0.76
1:A:639:PHE:HA	1:A:643:VAL:CG1	2.15	0.76
3:B:2236:1TP:C15	3:B:2236:1TP:H2	2.12	0.75
1:A:1231:LYS:HG3	1:A:1232:LYS:N	1.99	0.75
1:A:644:LYS:HB3	1:A:645:PRO:HD3	1.69	0.75
1:A:239:VAL:HG23	1:A:240:PRO:HD3	1.67	0.74
1:A:730:GLU:CD	1:A:730:GLU:H	1.93	0.74
1:A:14:THR:HG22	1:A:149:ALA:HB1	1.69	0.74
1:A:239:VAL:CG2	1:A:240:PRO:HD3	2.18	0.74
1:A:10:GLY:O	1:A:14:THR:HG23	1.86	0.74
1:A:561:MET:HE1	1:A:583:LEU:HD11	1.70	0.73
1:A:1102:ASP:OD1	1:A:1104:ARG:HG2	1.87	0.73
1:A:110:HIS:HD2	1:A:169:HIS:CD2	2.05	0.73
1:B:1198:ASP:OD2	1:B:1200:THR:HB	1.90	0.71
1:B:591:TYR:C	1:B:593:LYS:H	1.97	0.71
1:B:1219:THR:HG22	1:B:1221:GLU:H	1.54	0.71
1:B:598:ILE:HD13	1:B:601:MET:CE	2.20	0.70
1:A:708:LEU:HD21	1:A:731:LEU:HD22	1.74	0.70
1:A:1198:ASP:OD2	1:A:1200:THR:HB	1.91	0.70
1:A:731:LEU:HD23	1:A:790:VAL:HG11	1.73	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:140:MET:HE3	1:B:168:MET:CE	2.20	0.70
1:A:1230:THR:O	1:A:1232:LYS:HG2	1.92	0.70
1:B:1200:THR:CG2	1:B:1202:MET:H	1.99	0.69
1:B:635:THR:CG2	1:B:639:PHE:HB3	2.22	0.69
1:A:110:HIS:CD2	1:A:169:HIS:HD2	2.11	0.69
1:A:123:ILE:HD13	1:B:1202:MET:HE2	1.74	0.69
1:A:731:LEU:CD2	1:A:790:VAL:HG11	2.21	0.69
1:B:730:GLU:H	1:B:730:GLU:CD	2.01	0.69
1:A:1200:THR:CG2	1:A:1202:MET:H	2.03	0.68
1:B:731:LEU:HD23	1:B:790:VAL:HG11	1.75	0.68
1:B:1102:ASP:OD1	1:B:1104:ARG:HG2	1.92	0.68
1:A:163:SER:HB2	1:A:239:VAL:HG12	1.75	0.68
1:B:691:GLN:HG2	1:B:736:PHE:CD2	2.29	0.67
1:A:483:ARG:HG2	1:A:483:ARG:HH11	1.59	0.67
1:B:41:ASP:HA	1:B:58:ILE:HD12	1.77	0.67
1:A:593:LYS:HG3	1:A:594:LYS:N	2.10	0.67
3:B:2236:1TP:C2	3:B:2236:1TP:C7'	2.71	0.67
1:B:630:LYS:HB2	1:B:632:GLU:HG3	1.77	0.66
1:A:558:ARG:HG2	1:A:560:ASN:HD21	1.61	0.66
1:A:1006:PRO:HG2	1:A:1009:ALA:HB2	1.76	0.66
1:A:467:HIS:HD2	1:A:481:VAL:H	1.41	0.66
1:A:635:THR:HG23	1:A:672:PHE:CG	2.30	0.66
1:B:140:MET:HE3	1:B:168:MET:HE1	1.76	0.66
1:A:431:VAL:CG2	1:A:464:THR:HG21	2.26	0.66
1:B:731:LEU:HD21	1:B:790:VAL:HG11	1.78	0.66
1:A:467:HIS:CD2	1:A:481:VAL:H	2.14	0.65
1:A:971:TYR:OH	1:A:1028:MET:HE2	1.96	0.65
1:B:713:GLU:OE1	1:B:785:PRO:HD2	1.97	0.65
1:A:877:PHE:CE1	1:A:982:GLU:HG3	2.26	0.65
1:A:97:MET:HE1	1:A:168:MET:HE3	1.80	0.64
1:A:1219:THR:HG22	1:A:1221:GLU:H	1.61	0.64
1:A:1033:GLY:C	1:A:1175:PHE:HZ	2.05	0.64
1:B:110:HIS:HE1	1:B:157:HIS:NE2	1.95	0.64
1:A:602:ASN:O	1:A:606:VAL:HG23	1.99	0.63
1:A:1231:LYS:CG	1:A:1232:LYS:H	2.11	0.63
1:B:140:MET:HG2	1:B:168:MET:HE2	1.79	0.62
1:A:121:LEU:HD23	1:A:121:LEU:C	2.23	0.62
1:B:1219:THR:HG22	1:B:1221:GLU:N	2.14	0.62
3:A:2236:1TP:C25	3:A:2236:1TP:C35	2.74	0.62
1:B:907:LYS:O	1:B:911:GLN:HG3	2.00	0.62
1:A:1202:MET:HE2	1:B:123:ILE:HD13	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:708:LEU:HD21	1:B:731:LEU:HD22	1.82	0.62
1:A:636:ASN:ND2	1:A:639:PHE:H	1.99	0.61
1:A:1156:LEU:HD12	1:A:1157:ASP:N	2.16	0.61
1:A:937:GLN:HG2	1:A:942:LEU:HB3	1.83	0.61
1:A:1219:THR:HG22	1:A:1221:GLU:N	2.14	0.61
1:A:445:THR:HG21	1:A:574:LEU:HD21	1.83	0.60
1:A:591:TYR:C	1:A:593:LYS:H	2.08	0.60
1:A:686:PRO:HB2	1:A:724:LEU:HD21	1.82	0.60
1:B:775:VAL:O	1:B:779:GLU:HG2	2.00	0.60
1:A:881:MET:HE3	1:B:59:ARG:HG2	1.83	0.60
1:B:1200:THR:CG2	1:B:1202:MET:HB2	2.31	0.60
1:A:349:VAL:HG21	1:B:345:CYS:SG	2.41	0.60
1:A:691:GLN:HG2	1:A:736:PHE:CD2	2.36	0.60
1:A:2:GLY:N	1:A:187:ASP:OD2	2.35	0.60
1:B:239:VAL:HB	1:B:240:PRO:HD3	1.83	0.60
1:A:549:ILE:HG23	1:A:608:GLN:HG2	1.84	0.59
1:A:832:MET:HE2	1:A:834:ILE:HD11	1.85	0.59
1:B:1200:THR:HG21	1:B:1202:MET:HB2	1.85	0.59
1:A:14:THR:HG21	1:A:171:PHE:CE2	2.38	0.58
1:B:992:GLU:O	1:B:993:VAL:HG13	2.03	0.58
1:A:936:GLY:O	1:A:938:LYS:HD3	2.04	0.58
1:B:110:HIS:CD2	1:B:169:HIS:CD2	2.79	0.58
1:A:609:ALA:O	1:A:613:LEU:HB2	2.03	0.58
1:A:163:SER:O	1:A:164:ASN:HB2	2.04	0.58
1:A:243:VAL:O	1:A:247:MET:HG3	2.03	0.58
1:A:1051:LYS:HE3	1:A:1100:ARG:NH1	2.19	0.58
1:A:434:ASN:ND2	1:A:466:SER:OG	2.37	0.58
1:A:441:ILE:HD13	1:A:573:VAL:HG21	1.86	0.57
1:A:24:VAL:HG13	1:B:881:MET:HE2	1.85	0.57
1:A:61:MET:HG3	1:A:67:ALA:HA	1.85	0.57
1:A:976:HIS:HD2	1:B:1003:LYS:NZ	2.01	0.57
1:A:1188:PHE:CE1	1:A:1196:THR:HG23	2.39	0.57
1:A:1077:ARG:HG2	1:A:1130:ALA:O	2.05	0.57
1:A:739:GLN:NE2	1:A:777:ASN:HB3	2.20	0.57
1:A:881:MET:HE2	1:B:24:VAL:HG13	1.86	0.57
1:A:635:THR:HG23	1:A:672:PHE:CD2	2.40	0.57
1:B:61:MET:HG3	1:B:67:ALA:HA	1.85	0.57
1:A:1226:LEU:O	1:A:1230:THR:HG22	2.05	0.56
1:B:1232:LYS:HB3	1:B:1232:LYS:HZ2	1.70	0.56
1:B:1200:THR:CG2	1:B:1202:MET:HE3	2.30	0.56
1:A:1188:PHE:HE1	1:A:1196:THR:HG23	1.71	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:497:ILE:HG13	1:B:498:TYR:CD1	2.40	0.56
1:B:7:THR:HG21	1:B:439:LYS:HA	1.86	0.56
1:A:56:LEU:HD23	1:A:58:ILE:HD11	1.87	0.56
1:B:729:LYS:O	1:B:732:LYS:HG3	2.05	0.56
1:A:142:ALA:HB2	1:A:170:PHE:CZ	2.41	0.56
1:A:522:MET:SD	1:A:526:LEU:HD22	2.46	0.56
1:A:635:THR:HG22	1:A:636:ASN:N	2.12	0.56
1:B:483:ARG:HA	1:B:503:GLY:O	2.05	0.56
1:A:1123:SER:O	1:A:1126:GLU:HG2	2.06	0.56
1:A:1200:THR:HG23	1:A:1201:PRO:HD2	1.87	0.56
1:A:635:THR:HG21	1:A:639:PHE:CG	2.40	0.55
1:B:591:TYR:O	1:B:593:LYS:N	2.38	0.55
1:A:110:HIS:HE1	1:A:157:HIS:NE2	2.04	0.55
1:A:774:GLN:HA	1:A:777:ASN:HB2	1.88	0.55
1:B:803:GLU:OE1	1:B:856:ASN:HB2	2.07	0.55
1:A:14:THR:CG2	1:A:149:ALA:HB1	2.36	0.55
1:B:896:LYS:HB2	1:B:941:LEU:HD21	1.87	0.55
1:B:1182:ALA:O	1:B:1183:ASP:C	2.49	0.55
1:A:411:ASP:HB2	1:A:483:ARG:HD2	1.88	0.55
1:A:421:GLN:HA	1:A:466:SER:O	2.05	0.55
1:A:1171:ILE:HD12	1:B:1161:LYS:HD3	1.89	0.55
1:A:20:ALA:HB2	1:A:188:TYR:CE1	2.42	0.55
1:A:992:GLU:O	1:A:993:VAL:HG13	2.07	0.55
3:B:2236:1TP:N3	3:B:2236:1TP:H2	2.04	0.55
1:A:692:CYS:O	1:A:693:ASN:HB2	2.06	0.54
1:B:591:TYR:C	1:B:593:LYS:N	2.63	0.54
1:B:1219:THR:HG22	1:B:1220:SER:N	2.22	0.54
1:B:42:ASP:O	1:B:46:GLN:HG3	2.07	0.54
1:B:1027:ARG:HA	1:B:1030:MET:HE3	1.89	0.54
1:A:242:ILE:O	1:A:245:GLU:HG2	2.07	0.54
1:B:121:LEU:C	1:B:121:LEU:HD23	2.32	0.54
1:A:591:TYR:C	1:A:593:LYS:N	2.64	0.54
1:A:1176:ALA:HB1	1:A:1177:PRO:HD2	1.90	0.54
1:A:737:ARG:HE	1:A:739:GLN:NE2	2.05	0.54
1:A:766:PRO:HB2	1:A:769:THR:HG23	1.90	0.54
1:A:221:ASN:HB3	1:A:222:PRO:CD	2.38	0.53
1:A:483:ARG:HG2	1:A:483:ARG:NH1	2.24	0.53
1:A:99:LYS:HE3	1:B:867:SER:O	2.08	0.53
1:A:1219:THR:CG2	1:A:1221:GLU:H	2.21	0.53
1:B:27:ILE:HD12	1:B:1013:PHE:CE2	2.43	0.53
1:A:841:SER:HA	1:A:844:TRP:CE2	2.44	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:779:GLU:HB3	1:B:783:ARG:HH21	1.74	0.53
1:B:1219:THR:CG2	1:B:1220:SER:N	2.71	0.53
1:A:455:TYR:HB2	1:B:1201:PRO:HD3	1.90	0.53
1:B:1232:LYS:HB3	1:B:1232:LYS:NZ	2.23	0.53
1:B:691:GLN:O	1:B:797:LYS:HE3	2.09	0.53
1:A:1166:MET:O	1:A:1169:THR:HG22	2.08	0.52
1:A:805:LEU:HB2	1:A:825:THR:HB	1.91	0.52
1:A:180:ILE:O	1:A:450:GLN:HA	2.09	0.52
1:A:1200:THR:CG2	1:A:1202:MET:HB2	2.39	0.52
1:B:841:SER:HA	1:B:844:TRP:CE2	2.44	0.52
1:A:221:ASN:HB3	1:A:222:PRO:HD2	1.92	0.52
1:A:976:HIS:HD2	1:B:1003:LYS:HZ2	1.56	0.52
1:A:389:HIS:HE1	1:B:350:GLU:OE1	1.91	0.52
1:A:635:THR:HG21	1:A:639:PHE:HB3	1.91	0.52
1:B:221:ASN:HB3	1:B:222:PRO:CD	2.40	0.52
1:A:239:VAL:HG23	1:A:240:PRO:CD	2.37	0.51
1:A:341:TYR:CD1	1:A:360:ALA:HB2	2.46	0.51
1:A:6:MET:HE2	1:A:8:THR:HG21	1.92	0.51
1:A:239:VAL:CG2	1:A:307:PRO:HG2	2.40	0.51
3:A:2236:1TP:O35	1:B:1202:MET:HG2	2.11	0.51
1:A:523:ASP:HA	1:A:531:LYS:NZ	2.25	0.51
1:A:20:ALA:HB2	1:A:188:TYR:CZ	2.45	0.51
1:A:593:LYS:HG3	1:A:594:LYS:H	1.74	0.51
1:A:1189:GLY:CA	1:A:1196:THR:HG21	2.40	0.51
1:A:1000:GLN:HA	1:A:1012:LYS:HB2	1.93	0.50
1:B:590:ALA:O	1:B:591:TYR:C	2.51	0.50
1:A:317:LEU:HD21	1:A:324:ILE:HD11	1.93	0.50
1:A:1155:GLU:HG2	1:B:1173:GLU:OE2	2.12	0.50
1:A:1230:THR:O	1:A:1231:LYS:C	2.55	0.50
1:B:91:LEU:HD11	1:B:116:ILE:HD12	1.93	0.50
1:B:1012:LYS:O	1:B:1013:PHE:HB2	2.11	0.50
1:A:558:ARG:HG2	1:A:560:ASN:ND2	2.25	0.50
1:A:43:TRP:HB3	1:A:48:ARG:HD3	1.93	0.50
1:A:1051:LYS:HE3	1:A:1100:ARG:CZ	2.42	0.49
1:A:739:GLN:HE22	1:A:777:ASN:HB3	1.77	0.49
1:A:385:ALA:O	1:A:386:LYS:HB2	2.13	0.49
1:A:1156:LEU:HD12	1:A:1156:LEU:C	2.38	0.49
1:B:210:PRO:O	1:B:213:PRO:HD3	2.11	0.49
1:B:598:ILE:HD13	1:B:601:MET:HE1	1.94	0.49
1:B:896:LYS:CB	1:B:941:LEU:HD21	2.41	0.49
1:B:1225:ASP:O	1:B:1229:ARG:HG3	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:565:THR:HG21	1:A:609:ALA:HB3	1.93	0.49
1:A:955:LYS:HD2	1:B:210:PRO:HG3	1.94	0.49
1:A:976:HIS:HE1	1:B:60:GLU:O	1.95	0.49
1:B:5:MET:SD	1:B:184:GLU:HG2	2.52	0.49
1:A:949:SER:HA	1:A:952:TYR:CE2	2.48	0.49
1:A:635:THR:CG2	1:A:639:PHE:HB3	2.42	0.49
1:A:964:GLY:O	1:A:968:ASP:HB2	2.13	0.49
1:A:1094:GLY:HA3	1:A:1120:PRO:HG3	1.95	0.49
1:A:124:PHE:HB3	1:A:367:SER:HB2	1.96	0.48
1:A:212:HIS:HE1	1:B:950:ASP:OD2	1.96	0.48
1:A:635:THR:HG21	1:A:639:PHE:CB	2.43	0.48
1:A:1200:THR:HG21	1:A:1202:MET:HB2	1.95	0.48
1:B:779:GLU:HB3	1:B:783:ARG:NH2	2.28	0.48
1:B:522:MET:SD	1:B:526:LEU:HD13	2.53	0.48
1:B:936:GLY:O	1:B:938:LYS:HG2	2.13	0.48
1:B:1231:LYS:HG3	1:B:1232:LYS:N	2.29	0.48
1:B:1231:LYS:HG3	1:B:1232:LYS:H	1.78	0.48
1:A:1165:HIS:NE2	1:B:1165:HIS:CD2	2.82	0.48
1:B:805:LEU:HB2	1:B:825:THR:HB	1.95	0.48
1:A:345:CYS:O	1:A:349:VAL:HG13	2.14	0.48
1:A:526:LEU:O	1:A:531:LYS:HE3	2.13	0.48
1:A:1219:THR:HG21	6:B:2298:HOH:O	2.14	0.48
1:B:598:ILE:HA	1:B:601:MET:HE3	1.96	0.48
1:A:950:ASP:OD2	1:B:212:HIS:HE1	1.97	0.48
1:B:124:PHE:HB3	1:B:367:SER:HB2	1.95	0.48
1:B:499:ASP:OD2	1:B:502:GLU:HB2	2.14	0.48
1:A:593:LYS:CG	1:A:594:LYS:H	2.24	0.48
1:A:1165:HIS:CD2	1:B:1165:HIS:NE2	2.82	0.48
1:A:698:VAL:HG13	6:A:2217:HOH:O	2.13	0.47
1:A:805:LEU:HD12	1:A:829:GLY:HA3	1.96	0.47
1:A:9:ASP:HA	1:A:179:GLU:O	2.14	0.47
1:A:931:LYS:HE2	1:A:949:SER:HB2	1.95	0.47
1:A:994:TYR:HD2	3:A:2236:1TP:H5A1	1.78	0.47
1:B:243:VAL:O	1:B:247:MET:HG3	2.14	0.47
1:B:766:PRO:HB2	1:B:769:THR:HG23	1.94	0.47
1:A:667:LEU:HB3	1:A:854:LYS:HA	1.95	0.47
1:A:1015:ALA:CB	1:B:1185:SER:HB2	2.44	0.47
1:B:1156:LEU:C	1:B:1156:LEU:HD12	2.39	0.47
1:A:1209:GLY:O	1:B:429:GLY:HA2	2.14	0.47
1:B:9:ASP:HA	1:B:179:GLU:O	2.14	0.47
1:A:995:SER:O	1:B:1203:MET:HE2	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:516:TRP:O	1:A:522:MET:HE2	2.14	0.47
1:B:581:ASP:O	1:B:585:LYS:HG2	2.15	0.47
1:A:59:ARG:CG	1:B:881:MET:HE3	2.44	0.47
1:B:561:MET:HE1	1:B:583:LEU:CD2	2.40	0.47
1:B:673:GLU:O	1:B:674:LYS:C	2.57	0.47
1:A:434:ASN:ND2	1:A:466:SER:CB	2.78	0.46
1:A:499:ASP:OD2	1:A:502:GLU:HB2	2.16	0.46
1:B:630:LYS:HG3	1:B:632:GLU:OE2	2.15	0.46
1:A:222:PRO:HD3	1:B:124:PHE:CE2	2.50	0.46
1:A:351:ARG:HD3	1:A:353:GLU:HB2	1.97	0.46
1:A:467:HIS:C	1:A:468:LEU:HD23	2.40	0.46
1:A:730:GLU:CD	1:A:730:GLU:N	2.70	0.46
1:A:1189:GLY:HA3	1:A:1196:THR:HG21	1.98	0.46
1:A:483:ARG:HA	1:A:503:GLY:O	2.14	0.46
1:B:701:HIS:CE1	1:B:746:MET:HG3	2.51	0.46
1:A:1227:SER:HA	1:A:1230:THR:HG22	1.96	0.46
1:A:520:GLU:HG3	1:A:521:ASP:N	2.30	0.46
1:A:297:ILE:HB	1:A:379:TYR:CE2	2.51	0.46
1:A:59:ARG:HG2	1:B:881:MET:HE3	1.97	0.46
1:A:1068:TYR:HD1	1:A:1096:TRP:CE3	2.33	0.46
1:B:632:GLU:O	1:B:632:GLU:CD	2.59	0.46
1:A:116:ILE:HD11	1:A:129:ASP:HB3	1.98	0.46
1:A:233:ASN:HB2	1:A:234:PRO:HD3	1.97	0.46
1:B:1180:GLY:O	1:B:1182:ALA:N	2.38	0.46
1:A:873:ALA:HA	1:A:959:ILE:HD13	1.98	0.45
1:A:496:GLY:HA2	1:A:527:PRO:HG2	1.97	0.45
1:A:949:SER:HA	1:A:952:TYR:CZ	2.51	0.45
1:B:290:LEU:HD21	1:B:376:LYS:HD3	1.98	0.45
1:B:532:ARG:NH1	1:B:625:ALA:O	2.47	0.45
1:B:1077:ARG:HG3	1:B:1130:ALA:O	2.17	0.45
1:A:580:VAL:O	1:A:584:LYS:HG3	2.16	0.45
1:A:1232:LYS:NZ	1:A:1232:LYS:HB3	2.31	0.45
1:B:675:ARG:HD3	6:B:2271:HOH:O	2.16	0.45
1:A:110:HIS:CD2	1:A:169:HIS:CD2	2.94	0.45
1:A:635:THR:HG21	1:A:639:PHE:CD2	2.52	0.44
1:B:428:ASP:C	1:B:428:ASP:OD1	2.60	0.44
1:B:56:LEU:HD23	1:B:58:ILE:HD11	1.98	0.44
1:A:701:HIS:CE1	1:A:746:MET:HG3	2.52	0.44
1:A:881:MET:HE3	1:B:59:ARG:CG	2.46	0.44
1:A:1124:VAL:O	1:A:1127:PHE:HB3	2.18	0.44
1:B:997:THR:HG21	3:B:2236:1TP:H4A3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:590:ALA:O	1:A:591:TYR:C	2.60	0.44
1:B:460:SER:HB3	1:B:746:MET:CE	2.47	0.44
1:A:1219:THR:CG2	1:A:1220:SER:N	2.81	0.44
1:A:27:ILE:CD1	1:A:1013:PHE:CE2	2.96	0.44
1:A:1028:MET:CE	6:B:2373:HOH:O	2.65	0.44
1:B:467:HIS:CE1	1:B:480:LEU:HB3	2.53	0.43
1:B:670:SER:HA	1:B:673:GLU:OE1	2.17	0.43
1:B:730:GLU:CD	1:B:730:GLU:N	2.74	0.43
1:A:764:MET:C	1:A:765:GLN:HG2	2.43	0.43
1:A:1015:ALA:HB3	1:B:1185:SER:HB2	1.99	0.43
1:A:1077:ARG:HG2	1:A:1130:ALA:C	2.42	0.43
6:A:2024:HOH:O	1:B:871:ASP:HB3	2.17	0.43
1:B:20:ALA:HB2	1:B:188:TYR:CZ	2.53	0.43
1:B:131:TYR:CE2	1:B:339:PRO:HB2	2.53	0.43
1:A:643:VAL:O	1:A:647:LEU:HG	2.17	0.43
1:A:1219:THR:HG22	1:A:1222:GLN:H	1.82	0.43
1:B:240:PRO:HB3	1:B:309:VAL:HG21	2.00	0.43
1:B:828:PHE:CE2	1:B:1057:GLU:HG3	2.53	0.43
1:B:1000:GLN:H	1:B:1000:GLN:NE2	2.16	0.43
1:A:1180:GLY:O	1:A:1181:LYS:HB2	2.18	0.43
1:B:808:PHE:N	1:B:808:PHE:CD2	2.85	0.43
1:B:1006:PRO:HG3	1:B:1095:TYR:OH	2.19	0.43
1:B:667:LEU:HB3	1:B:854:LYS:HA	2.00	0.43
1:A:422:PHE:O	1:A:465:ILE:HA	2.17	0.43
1:A:534:ILE:HG23	1:A:539:LEU:HB2	2.00	0.43
1:B:110:HIS:CE1	1:B:157:HIS:NE2	2.80	0.43
1:A:361:GLY:HA3	1:A:390:PHE:CZ	2.53	0.43
1:A:586:SER:O	1:A:589:LYS:HB3	2.18	0.43
1:A:1028:MET:HE3	6:B:2373:HOH:O	2.17	0.43
1:B:1105:LEU:HD23	1:B:1105:LEU:HA	1.84	0.43
1:A:591:TYR:O	1:A:593:LYS:N	2.51	0.43
1:B:589:LYS:HE2	1:B:589:LYS:HB3	1.76	0.43
1:A:131:TYR:CE2	1:A:339:PRO:HB2	2.54	0.42
1:B:1166:MET:O	1:B:1169:THR:HG22	2.19	0.42
1:A:840:CYS:HB2	3:A:2236:1TP:O22	2.20	0.42
1:A:97:MET:HE1	1:A:168:MET:CE	2.46	0.42
1:A:429:GLY:HA2	1:B:1209:GLY:O	2.18	0.42
1:A:953:THR:HG22	6:A:2294:HOH:O	2.19	0.42
1:A:87:SER:HA	1:A:129:ASP:HB3	2.00	0.42
1:A:677:VAL:O	1:B:1216:ARG:HD2	2.19	0.42
1:B:796:LEU:HA	1:B:1050:LEU:HD11	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:560:ASN:H	1:A:560:ASN:HD22	1.66	0.42
1:A:902:ALA:O	1:A:907:LYS:HE3	2.19	0.42
3:B:2236:1TP:C2	3:B:2236:1TP:C35	2.89	0.42
1:A:121:LEU:HD23	1:A:122:SER:N	2.35	0.42
1:A:497:ILE:HG13	1:A:498:TYR:CD1	2.54	0.42
1:A:700:PRO:HG2	1:A:814:GLY:HA2	2.01	0.42
1:A:1003:LYS:NZ	1:B:976:HIS:HD2	2.18	0.42
1:A:1203:MET:HE2	1:B:995:SER:O	2.19	0.42
1:A:808:PHE:CD2	1:A:808:PHE:N	2.85	0.42
1:A:953:THR:HG23	6:B:2077:HOH:O	2.19	0.42
1:A:126:ASP:OD2	1:A:126:ASP:C	2.63	0.42
1:A:1132:ASN:ND2	1:A:1136:VAL:HG13	2.34	0.42
1:B:27:ILE:HD12	1:B:1013:PHE:CZ	2.55	0.42
1:A:754:ILE:C	1:A:754:ILE:HD12	2.44	0.42
1:A:978:LEU:O	1:A:1062:PRO:HG2	2.20	0.42
1:A:1007:THR:OG1	1:A:1021:GLY:HA2	2.20	0.42
1:B:6:MET:HE2	1:B:185:VAL:HG11	2.02	0.42
1:B:635:THR:HG22	1:B:636:ASN:O	2.20	0.42
1:B:731:LEU:O	1:B:732:LYS:C	2.62	0.42
1:A:371:SER:HB2	1:A:372:PRO:CD	2.50	0.42
1:A:673:GLU:O	1:A:674:LYS:C	2.63	0.42
1:B:1076:LEU:HD13	1:B:1086:VAL:HG21	2.01	0.42
1:A:240:PRO:HB3	1:A:309:VAL:HG21	2.02	0.41
1:A:245:GLU:HG3	1:A:246:TYR:N	2.35	0.41
1:A:589:LYS:C	1:A:590:ALA:O	2.61	0.41
1:A:688:ASN:HB3	1:A:759:GLU:O	2.20	0.41
1:B:27:ILE:CD1	1:B:1013:PHE:CE2	3.04	0.41
1:B:67:ALA:O	1:B:71:VAL:HG23	2.20	0.41
1:B:978:LEU:O	1:B:1062:PRO:HG2	2.20	0.41
1:B:1046:LYS:HG3	6:B:2402:HOH:O	2.19	0.41
1:A:110:HIS:CE1	1:A:157:HIS:NE2	2.85	0.41
1:A:422:PHE:HE1	1:A:468:LEU:HG	1.85	0.41
1:A:562:ILE:HD12	1:A:562:ILE:N	2.34	0.41
1:B:1055:GLU:O	1:B:1104:ARG:NH1	2.52	0.41
1:A:1043:GLY:HA3	1:A:1084:GLN:O	2.21	0.41
1:B:1006:PRO:HG2	1:B:1009:ALA:HB2	2.03	0.41
1:A:266:ALA:HA	1:A:267:PRO:HD3	1.89	0.41
1:A:544:ILE:HG23	1:A:544:ILE:O	2.20	0.41
1:B:11:ASN:HD21	1:B:112:THR:HG21	1.85	0.41
1:B:80:LEU:HD23	1:B:80:LEU:HA	1.86	0.41
1:B:163:SER:O	1:B:164:ASN:HB2	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:126:ASP:HA	1:A:329:ARG:HD3	2.03	0.41
1:A:1200:THR:HG23	1:A:1201:PRO:CD	2.49	0.41
1:B:819:PRO:O	1:B:823:VAL:HG13	2.21	0.41
1:A:50:ASN:OD1	1:A:50:ASN:C	2.64	0.41
1:A:465:ILE:HG22	1:A:467:HIS:CE1	2.56	0.41
1:A:553:VAL:HG21	1:A:605:ALA:HB2	2.02	0.41
1:B:20:ALA:O	1:B:51:ILE:HG23	2.21	0.41
1:B:823:VAL:HG21	1:B:1049:PHE:CE2	2.56	0.41
1:B:961:GLY:HA3	1:B:965:TRP:CE3	2.55	0.41
1:B:587:ILE:O	1:B:590:ALA:O	2.39	0.41
1:B:786:VAL:HG12	1:B:801:PHE:O	2.21	0.41
1:B:832:MET:HE2	1:B:834:ILE:CG1	2.51	0.41
1:B:1104:ARG:HB2	6:B:2429:HOH:O	2.20	0.41
1:A:239:VAL:HG22	1:A:240:PRO:HD3	2.00	0.40
1:A:691:GLN:HG2	1:A:736:PHE:CE2	2.56	0.40
1:A:949:SER:C	1:A:951:LEU:H	2.29	0.40
1:A:1034:TYR:HB3	1:A:1175:PHE:CZ	2.57	0.40
1:A:422:PHE:HD1	1:A:466:SER:HB2	1.86	0.40
1:A:459:LYS:HB3	1:B:1198:ASP:HB2	2.02	0.40
1:A:1055:GLU:O	1:A:1104:ARG:NH1	2.53	0.40
1:B:439:LYS:HB2	1:B:439:LYS:NZ	2.36	0.40
1:B:686:PRO:HB2	1:B:724:LEU:HD21	2.04	0.40
1:A:114:ARG:NE	1:A:123:ILE:HA	2.36	0.40
1:A:132:ALA:HA	1:B:135:GLN:HE21	1.86	0.40
1:B:56:LEU:HG	1:B:58:ILE:HG12	2.02	0.40
1:B:832:MET:HE2	1:B:834:ILE:HD11	2.03	0.40
1:B:964:GLY:O	1:B:968:ASP:HB2	2.21	0.40
1:A:154:LEU:HD22	1:A:158:LEU:CD1	2.51	0.40
1:A:289:HIS:CE1	1:A:293:LYS:HE2	2.57	0.40
1:A:357:LYS:HE3	1:A:359:LEU:HD21	2.03	0.40
1:B:460:SER:HB3	1:B:746:MET:HE2	2.03	0.40
1:B:1119:ALA:O	1:B:1120:PRO:C	2.64	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries

of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1229/1231 (100%)	1168 (95%)	47 (4%)	14 (1%)	11	10
1	B	1229/1231 (100%)	1183 (96%)	40 (3%)	6 (0%)	24	26
All	All	2458/2462 (100%)	2351 (96%)	87 (4%)	20 (1%)	16	16

All (20) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	732	LYS
1	A	593	LYS
1	A	594	LYS
1	A	595	GLY
1	A	629	THR
1	A	630	LYS
1	B	629	THR
1	A	1178	ALA
1	A	1181	LYS
1	A	1182	ALA
1	A	1231	LYS
1	B	1183	ASP
1	B	591	TYR
1	A	87	SER
1	A	589	LYS
1	A	628	GLU
1	B	1182	ALA
1	B	1181	LYS
1	A	557	GLY
1	A	495	VAL

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	978/978 (100%)	937 (96%)	41 (4%)	26 34
1	B	978/978 (100%)	955 (98%)	23 (2%)	43 55
All	All	1956/1956 (100%)	1892 (97%)	64 (3%)	33 43

All (64) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	ASN
1	A	14	THR
1	A	154	LEU
1	A	194	LEU
1	A	198	LYS
1	A	204	ARG
1	A	211	GLU
1	A	317	LEU
1	A	327	LEU
1	A	349	VAL
1	A	351	ARG
1	A	365	LEU
1	A	399	THR
1	A	436	GLN
1	A	570	LEU
1	A	573	VAL
1	A	613	LEU
1	A	617	LYS
1	A	632	GLU
1	A	643	VAL
1	A	687	GLU
1	A	714	LEU
1	A	720	ASN
1	A	730	GLU
1	A	777	ASN
1	A	849	PRO
1	A	858	LEU
1	A	893	LEU
1	A	939	ASP
1	A	942	LEU
1	A	953	THR
1	A	982	GLU
1	A	1000	GLN
1	A	1104	ARG
1	A	1136	VAL

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Mol	Chain	Res	Type
1	A	1147	ARG
1	A	1170	ASN
1	A	1183	ASP
1	A	1196	THR
1	A	1219	THR
1	A	1232	LYS
1	B	194	LEU
1	B	290	LEU
1	B	317	LEU
1	B	342	LEU
1	B	359	LEU
1	B	439	LYS
1	B	463	ILE
1	B	509	THR
1	B	526	LEU
1	B	544	ILE
1	B	583	LEU
1	B	632	GLU
1	B	635	THR
1	B	714	LEU
1	B	725	GLU
1	B	730	GLU
1	B	754	ILE
1	B	823	VAL
1	B	836	ASN
1	B	849	PRO
1	B	931	LYS
1	B	1000	GLN
1	B	1232	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (50) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	11	ASN
1	A	46	GLN
1	A	110	HIS
1	A	128	GLN
1	A	169	HIS
1	A	212	HIS
1	A	289	HIS
1	A	389	HIS
1	A	434	ASN

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Mol	Chain	Res	Type
1	A	467	HIS
1	A	513	ASN
1	A	536	ASN
1	A	560	ASN
1	A	602	ASN
1	A	636	ASN
1	A	641	ASN
1	A	649	GLN
1	A	739	GLN
1	A	777	ASN
1	A	836	ASN
1	A	866	ASN
1	A	880	ASN
1	A	918	ASN
1	A	976	HIS
1	A	1000	GLN
1	A	1073	ASN
1	A	1088	ASN
1	A	1154	HIS
1	A	1170	ASN
1	B	11	ASN
1	B	46	GLN
1	B	96	ASN
1	B	110	HIS
1	B	128	GLN
1	B	169	HIS
1	B	212	HIS
1	B	434	ASN
1	B	543	ASN
1	B	608	GLN
1	B	688	ASN
1	B	777	ASN
1	B	937	GLN
1	B	976	HIS
1	B	996	ASN
1	B	1000	GLN
1	B	1047	GLN
1	B	1073	ASN
1	B	1088	ASN
1	B	1108	GLN
1	B	1154	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 12 ligands modelled in this entry, 4 are monoatomic - leaving 8 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	SF4	B	2234	1	0,12,12	-	-	-		
3	1TP	B	2236	4	27,33,33	4.55	14 (51%)	36,51,51	3.76	15 (41%)
2	SF4	A	2233	1	0,12,12	-	-	-		
2	SF4	B	2233	1	0,12,12	-	-	-		
2	SF4	B	2235	1	0,12,12	-	-	-		
3	1TP	A	2236	4	27,33,33	4.80	14 (51%)	36,51,51	2.98	14 (38%)
2	SF4	A	2234	1	0,12,12	-	-	-		
2	SF4	A	2235	1	0,12,12	-	-	-		

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	SF4	B	2234	1	-	-	0/6/5/5
2	SF4	A	2233	1	-	-	0/6/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	1TP	A	2236	4	1/1/8/8	11/24/45/45	0/2/2/2
2	SF4	B	2233	1	-	-	0/6/5/5
3	1TP	B	2236	4	1/1/8/8	8/24/45/45	0/2/2/2
2	SF4	B	2235	1	-	-	0/6/5/5
2	SF4	A	2234	1	-	-	0/6/5/5
2	SF4	A	2235	1	-	-	0/6/5/5

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	2236	1TP	C15-C25	13.36	1.82	1.53
3	A	2236	1TP	C15-C25	12.07	1.79	1.53
3	B	2236	1TP	C35-C15	10.93	1.71	1.52
3	A	2236	1TP	O25-C15	10.66	1.60	1.43
3	A	2236	1TP	O35-C25	8.91	1.50	1.22
3	B	2236	1TP	C2'-N1'	8.78	1.48	1.34
3	A	2236	1TP	C35-C15	8.10	1.66	1.52
3	A	2236	1TP	C2-S1	-7.61	1.68	1.83
3	B	2236	1TP	C5-S1	6.79	1.89	1.83
3	A	2236	1TP	C4A-C4	5.69	1.63	1.52
3	B	2236	1TP	C4'-N3'	4.95	1.42	1.35
3	A	2236	1TP	C4'-N3'	4.93	1.42	1.35
3	A	2236	1TP	C2'-N1'	4.15	1.41	1.34
3	B	2236	1TP	C5A-C5	4.15	1.62	1.52
3	A	2236	1TP	C5A-C5	4.10	1.62	1.52
3	B	2236	1TP	C7'-C5'	-3.83	1.45	1.51
3	B	2236	1TP	O45-C25	-3.79	1.16	1.30
3	A	2236	1TP	C6'-N1'	3.65	1.42	1.34
3	B	2236	1TP	P2-O23	-3.41	1.41	1.54
3	A	2236	1TP	P2-O21	3.23	1.61	1.50
3	B	2236	1TP	O5G-C5B	-3.13	1.31	1.44
3	A	2236	1TP	P2-O22	-3.08	1.43	1.54
3	A	2236	1TP	C7'-N3	2.67	1.51	1.47
3	B	2236	1TP	C2-S1	2.55	1.88	1.83
3	B	2236	1TP	P2-O22	-2.33	1.45	1.54
3	B	2236	1TP	O25-C15	2.31	1.46	1.43
3	B	2236	1TP	C2'-N3'	-2.21	1.30	1.34
3	A	2236	1TP	C2'-N3'	-2.04	1.30	1.34

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	2236	1TP	C2-S1-C5	-13.34	81.76	94.02
3	A	2236	1TP	C15-C2-N3	11.24	127.15	109.35
3	B	2236	1TP	C15-C2-N3	9.07	123.71	109.35
3	B	2236	1TP	C2A-C2'-N1'	7.94	125.88	117.14
3	B	2236	1TP	C4-C5-S1	6.79	114.88	104.81
3	A	2236	1TP	C2A-C2'-N1'	6.29	124.06	117.14
3	A	2236	1TP	N1'-C2'-N3'	-4.59	117.65	125.54
3	B	2236	1TP	N1'-C2'-N3'	-4.55	117.70	125.54
3	B	2236	1TP	C35-C15-C25	4.35	117.15	108.38
3	A	2236	1TP	C7'-N3-C4	4.20	122.40	114.45
3	A	2236	1TP	C2'-N3'-C4'	4.17	124.58	118.08
3	B	2236	1TP	C5A-C5-S1	-3.98	101.62	112.64
3	B	2236	1TP	O45-C25-O35	-3.93	111.31	123.82
3	A	2236	1TP	O5G-C5B-C5A	3.82	122.19	109.09
3	A	2236	1TP	C5A-C5-C4	-3.52	111.27	116.14
3	B	2236	1TP	C2'-N3'-C4'	3.43	123.43	118.08
3	B	2236	1TP	O5G-C5B-C5A	3.25	120.23	109.09
3	A	2236	1TP	C5A-C5-S1	-2.90	104.62	112.64
3	B	2236	1TP	O23-P2-O22	2.77	118.21	107.64
3	A	2236	1TP	C5'-C7'-N3	-2.76	108.19	113.17
3	A	2236	1TP	O23-P2-O22	2.53	117.32	107.64
3	A	2236	1TP	C6'-N1'-C2'	2.49	120.19	115.96
3	A	2236	1TP	C5'-C4'-N4'	2.39	125.58	122.19
3	A	2236	1TP	C7'-C5'-C4'	2.30	124.89	122.56
3	B	2236	1TP	C5A-C5-C4	-2.26	113.02	116.14
3	B	2236	1TP	N4'-C4'-N3'	-2.18	113.95	117.03
3	B	2236	1TP	C5'-C4'-N4'	2.17	125.26	122.19
3	A	2236	1TP	N4'-C4'-N3'	-2.11	114.05	117.03
3	B	2236	1TP	C6'-N1'-C2'	2.10	119.54	115.96

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	2236	1TP	C4
3	B	2236	1TP	C4

All (19) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	2236	1TP	S1-C5-C5A-C5B
3	A	2236	1TP	C4-C5-C5A-C5B
3	A	2236	1TP	C5-C5A-C5B-O5G
3	A	2236	1TP	P1-O11-P2-O23

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Mol	Chain	Res	Type	Atoms
3	B	2236	1TP	S1-C5-C5A-C5B
3	B	2236	1TP	C4-C5-C5A-C5B
3	B	2236	1TP	O25-C15-C25-O45
3	B	2236	1TP	C5'-C7'-N3-C4
3	A	2236	1TP	C35-C15-C25-O35
3	A	2236	1TP	O25-C15-C25-O45
3	A	2236	1TP	C5'-C7'-N3-C4
3	B	2236	1TP	O25-C15-C25-O35
3	A	2236	1TP	C5'-C7'-N3-C2
3	A	2236	1TP	C2-C15-C25-O35
3	B	2236	1TP	P1-O11-P2-O22
3	A	2236	1TP	C5B-O5G-P1-O11
3	B	2236	1TP	C5'-C7'-N3-C2
3	B	2236	1TP	C2-C15-C25-O35
3	A	2236	1TP	C5B-O5G-P1-O12

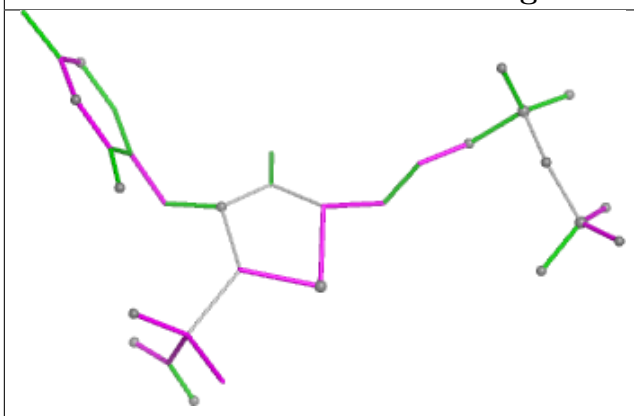
There are no ring outliers.

2 monomers are involved in 15 short contacts:

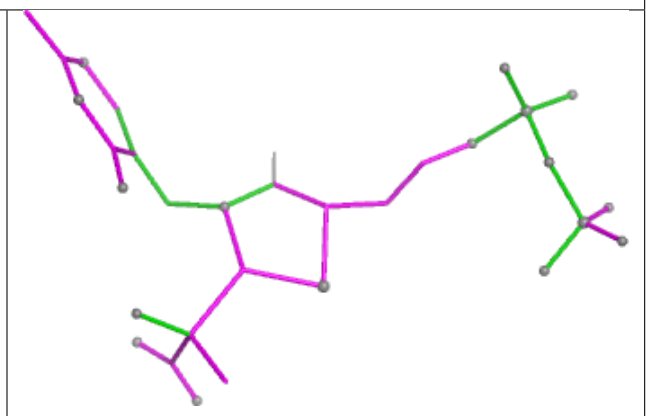
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	2236	1TP	8	0
3	A	2236	1TP	7	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

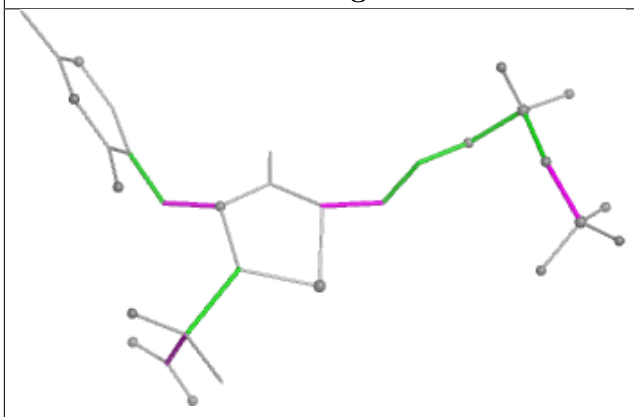
Ligand 1TP B 2236



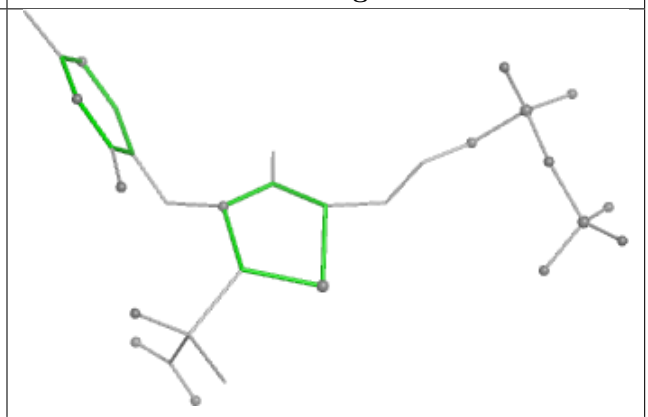
Bond lengths



Bond angles

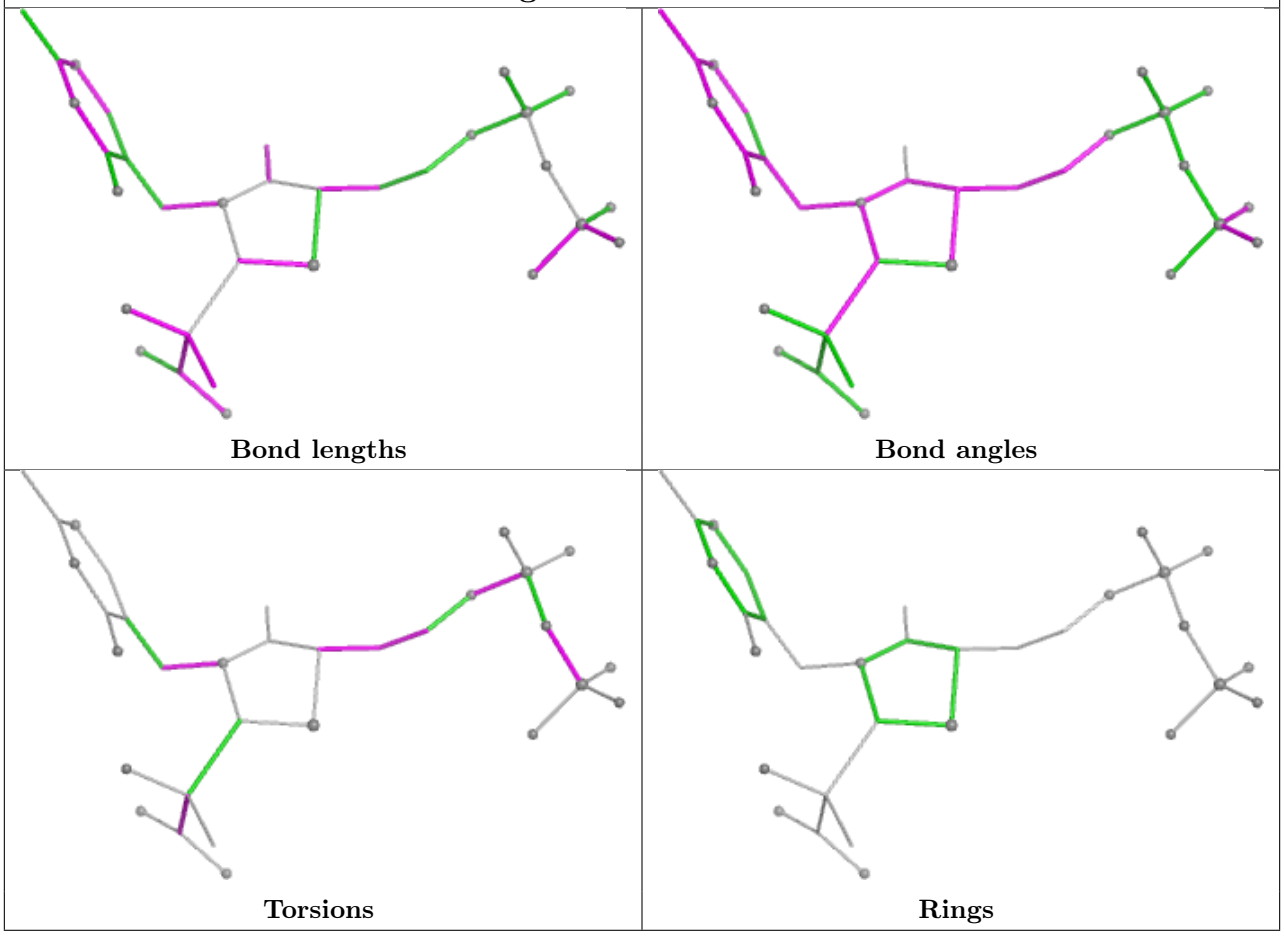


Torsions



Rings

Ligand 1TP A 2236



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	1231/1231 (100%)	-0.26	43 (3%)	47	53	7, 22, 62, 118	0
1	B	1231/1231 (100%)	-0.49	30 (2%)	59	65	7, 19, 46, 104	0
All	All	2462/2462 (100%)	-0.37	73 (2%)	52	59	7, 20, 57, 118	0

All (73) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1175	PHE	6.5
1	B	1178	ALA	6.2
1	A	1174	SER	6.2
1	A	1176	ALA	5.9
1	B	1175	PHE	5.9
1	A	1177	PRO	5.8
1	B	1176	ALA	5.7
1	A	1165	HIS	5.4
1	B	1181	LYS	4.9
1	A	1179	GLY	4.6
1	A	633	PRO	4.6
1	B	631	ALA	4.5
1	B	1165	HIS	4.4
1	B	1177	PRO	4.2
1	B	1174	SER	4.1
1	B	1179	GLY	4.0
1	A	1181	LYS	4.0
1	A	631	ALA	4.0
1	B	1180	GLY	4.0
1	A	595	GLY	4.0
1	A	1178	ALA	3.9
1	B	1183	ASP	3.8
1	B	629	THR	3.8
1	B	1173	GLU	3.7

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Mol	Chain	Res	Type	RSRZ
1	A	593	LYS	3.6
1	A	628	GLU	3.6
1	A	627	ALA	3.5
1	A	629	THR	3.4
1	B	593	LYS	3.4
1	B	1232	LYS	3.3
1	A	592	GLY	3.3
1	A	1180	GLY	3.3
1	A	591	TYR	3.3
1	A	1182	ALA	3.2
1	B	592	GLY	3.2
1	A	594	LYS	3.1
1	B	1231	LYS	3.1
1	A	635	THR	2.9
1	A	590	ALA	2.9
1	A	576	PHE	2.9
1	A	626	PRO	2.8
1	B	1182	ALA	2.8
1	B	595	GLY	2.8
1	A	1231	LYS	2.8
1	A	1232	LYS	2.8
1	B	627	ALA	2.7
1	A	497	ILE	2.7
1	A	1183	ASP	2.7
1	B	1230	THR	2.7
1	A	1173	GLU	2.7
1	A	1171	ILE	2.6
1	A	630	LYS	2.6
1	A	634	MET	2.5
1	A	1172	PHE	2.5
1	B	594	LYS	2.4
1	B	630	LYS	2.4
1	B	1172	PHE	2.4
1	A	619	PRO	2.4
1	B	591	TYR	2.3
1	B	633	PRO	2.3
1	A	598	ILE	2.3
1	B	634	MET	2.3
1	A	714	LEU	2.3
1	B	589	LYS	2.3
1	A	596	GLU	2.3
1	A	587	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	732	LYS	2.1
1	A	729	LYS	2.1
1	B	628	GLU	2.1
1	A	589	LYS	2.0
1	A	758	LYS	2.0
1	A	730	GLU	2.0
1	B	715	VAL	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates (i)

There are no oligosaccharides in this entry.

6.4 Ligands (i)

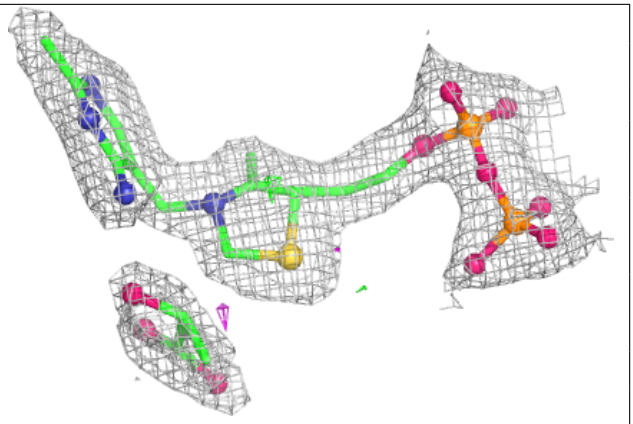
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

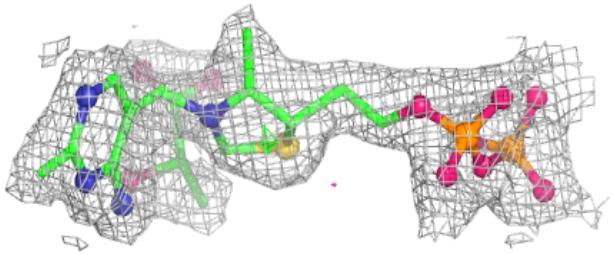
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	1TP	A	2236	32/32	0.98	0.07	14,20,39,43	0
5	CA	A	2238	1/1	0.98	0.24	57,57,57,57	0
2	SF4	A	2235	8/8	0.99	0.02	15,18,19,20	0
2	SF4	B	2233	8/8	0.99	0.03	19,20,21,23	0
2	SF4	B	2234	8/8	0.99	0.02	13,14,15,17	0
2	SF4	B	2235	8/8	0.99	0.03	10,12,13,13	0
2	SF4	A	2233	8/8	0.99	0.04	27,31,32,33	0
3	1TP	B	2236	32/32	0.99	0.05	6,15,32,32	0
2	SF4	A	2234	8/8	0.99	0.03	22,25,25,27	0
5	CA	B	2238	1/1	0.99	0.14	46,46,46,46	0
4	MG	A	2237	1/1	1.00	0.02	9,9,9,9	0
4	MG	B	2237	1/1	1.00	0.03	4,4,4,4	0

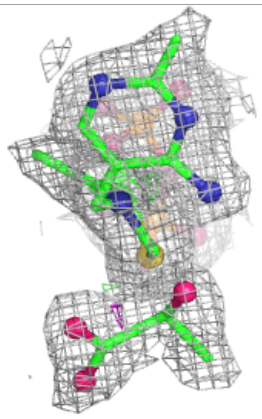
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around 1TP A 2236:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

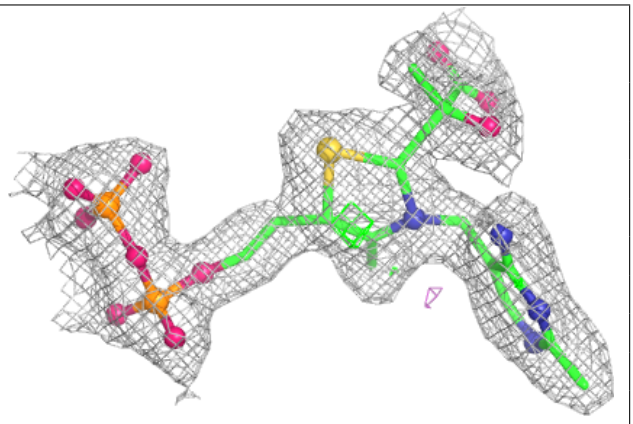


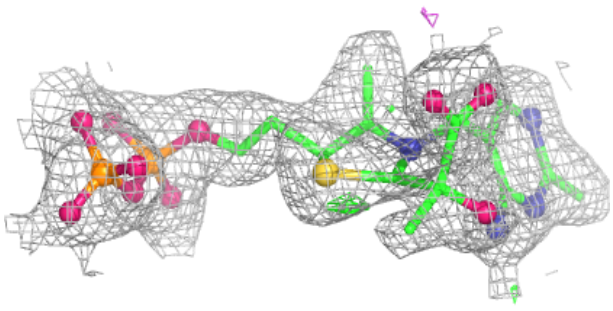


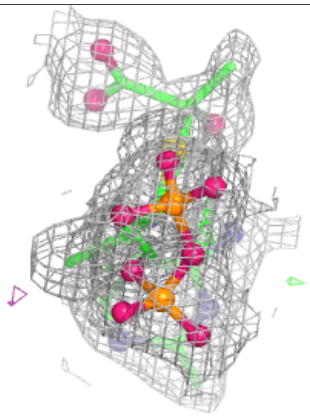


Electron density around 1TP B 2236:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)







6.5 Other polymers (i)

There are no such residues in this entry.